

3-Methyl-1-phenyl-1H-pyrazol-5-amine  
1131-18-6 | DTXSID6044517

Model Performance

|       |      |
|-------|------|
| Model | Data |
|-------|------|

| Weighted KNN model |      |                |      |            |      |
|--------------------|------|----------------|------|------------|------|
| 5-fold CV (75%)    |      | Training (75%) |      | Test (25%) |      |
| Q2                 | RMSE | R2             | RMSE | R2         | RMSE |
| 0.87               | 0.81 | 0.87           | 0.82 | 0.86       | 0.86 |

Model Results

Predicted value: 3.90e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 4.92e-01

Confidence level: 4.04e-01

Nearest Neighbors from the Training Set

|  |  |  |
|--|--|--|
| <div>Image not found</div> <div>1-Phenyl-2-thiourea</div> <div>Measured: 1.62e-02</div> <div>Predicted: 7.48e-02</div> | <div>Image not found</div> <div>Bis(ethylxanthogen)</div> <div>Measured: 1.14e-05</div> <div>Predicted: 4.06e-05</div> | <div>Image not found</div> <div>1,10-Phenanthroline</div> <div>Measured: 1.49e-02</div> <div>Predicted: 5.60e-03</div> |
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